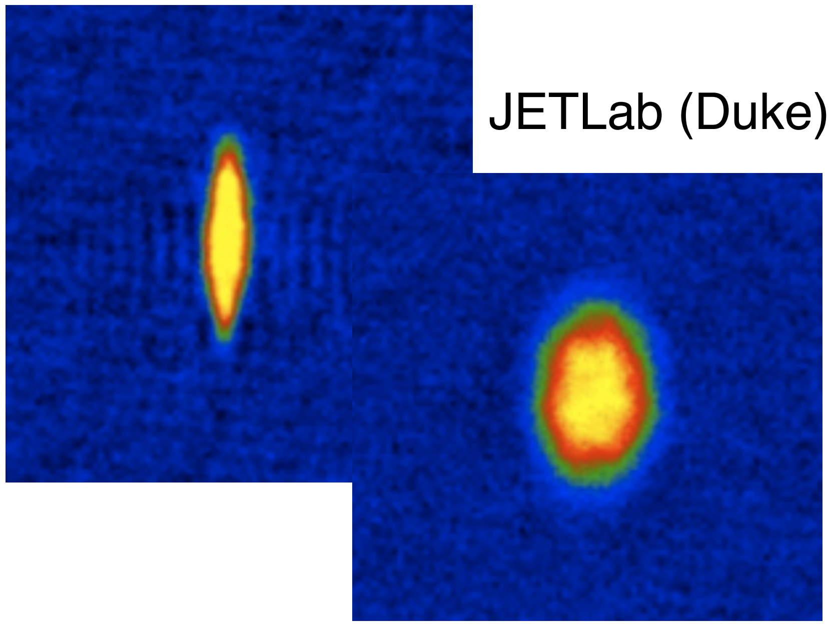
Improved lattice actions & operators for non-relativistic fermions

Joaquín E. Drut
Los Alamos National Laboratory

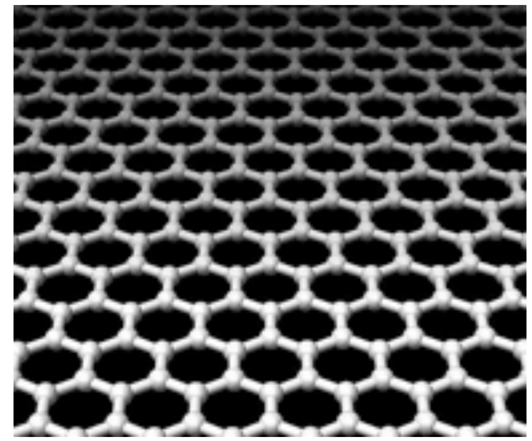
EMMI workshop
GSI, Darmstadt, April 2012

Ultracold Gases



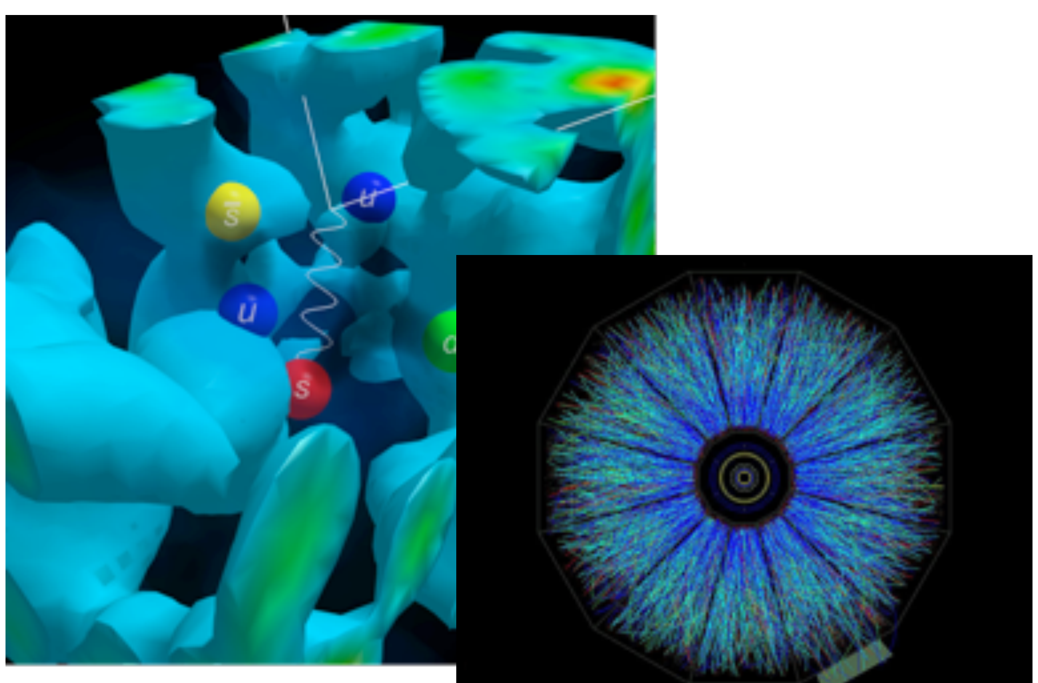
JETLab (Duke)

Condensed Matter Physics

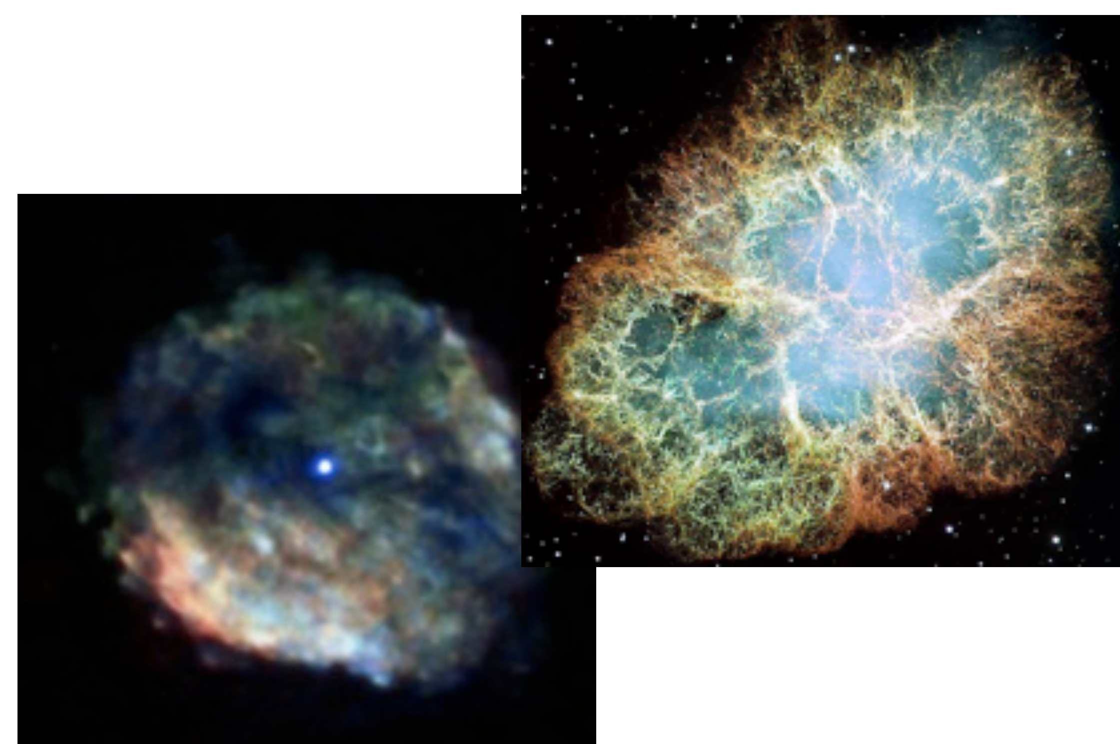


Materials Science

High-Energy Physics, QCD, Low-Energy NP



Astrophysics



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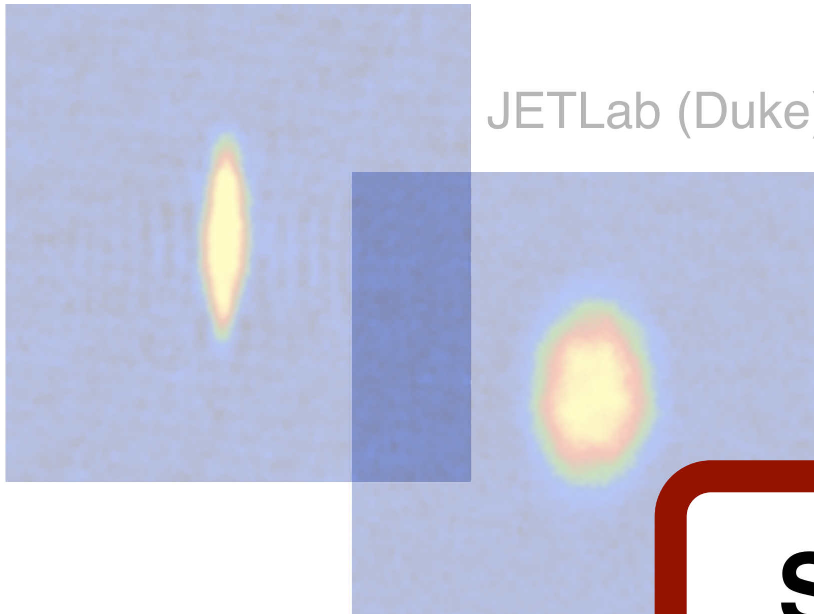

JETLab (Duke)

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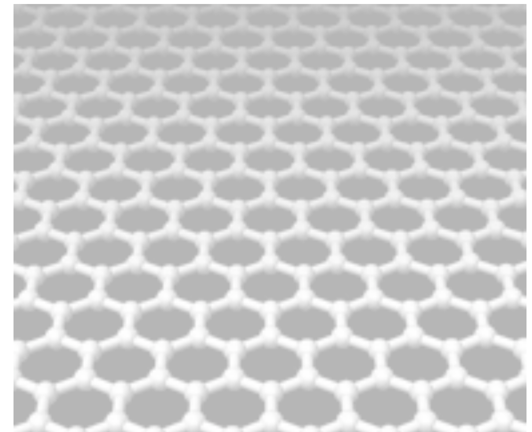
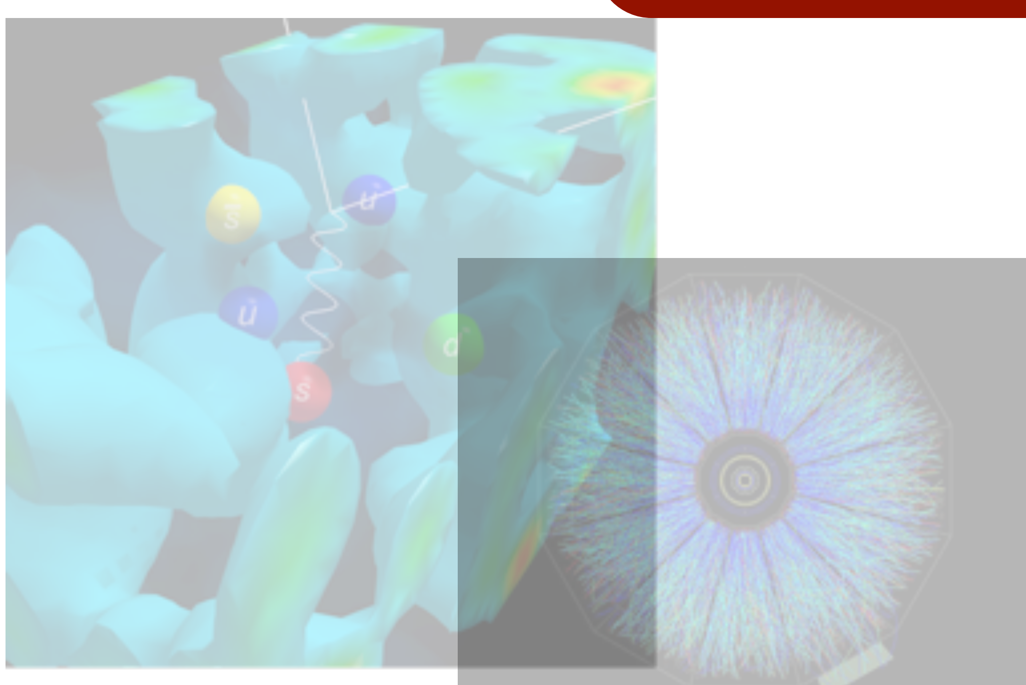


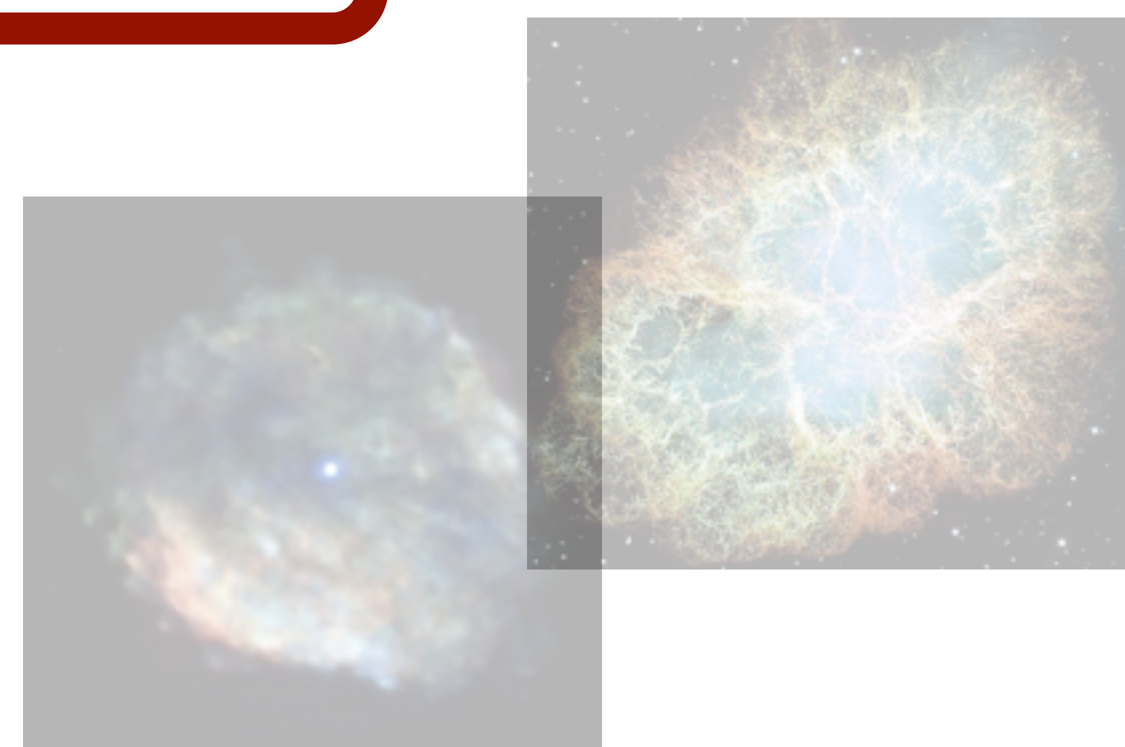
Materials Science

Strongly correlated quantum many-body systems

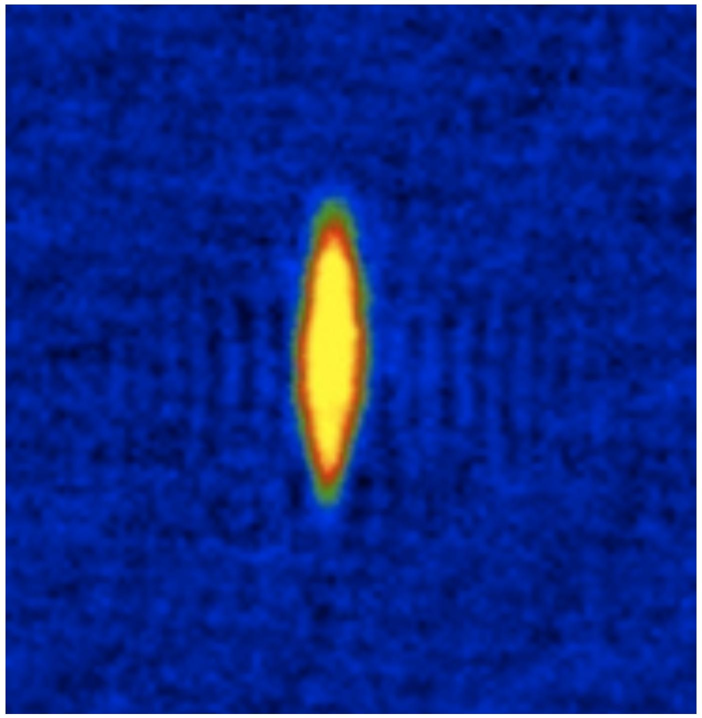
High-Energy Pl
QCD, Low-Ene



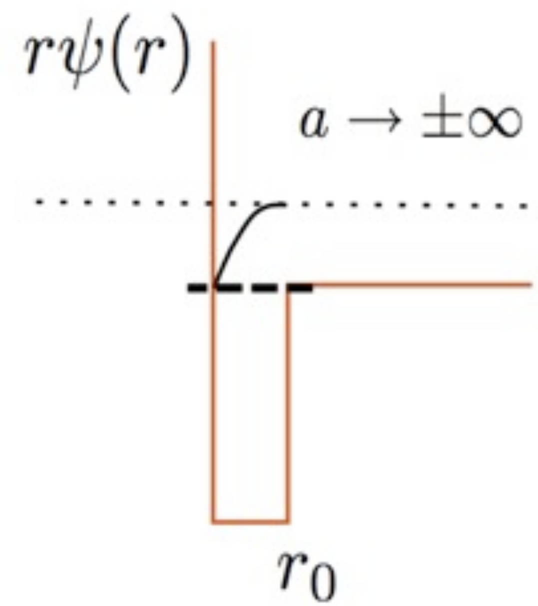
strophysics
ly neutron stars)

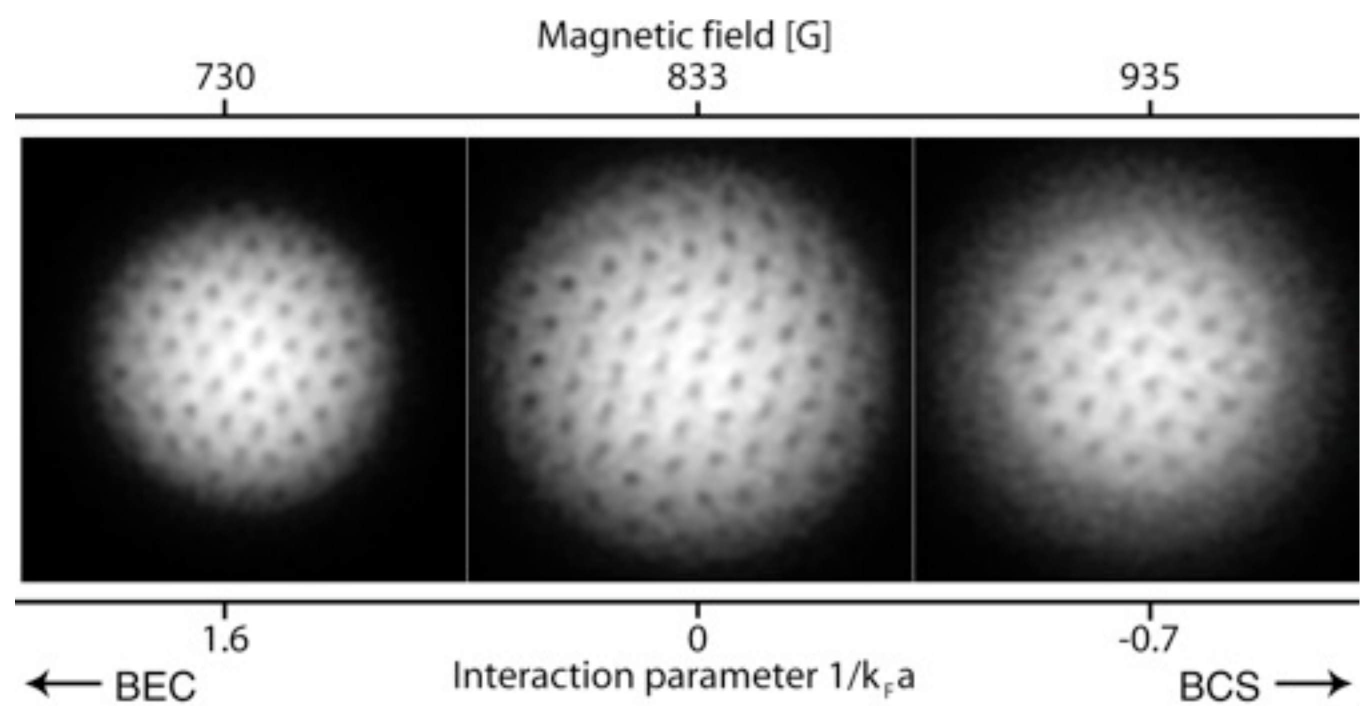


Ultracold Atoms



JET Lab (Duke)





MIT

The unitary limit

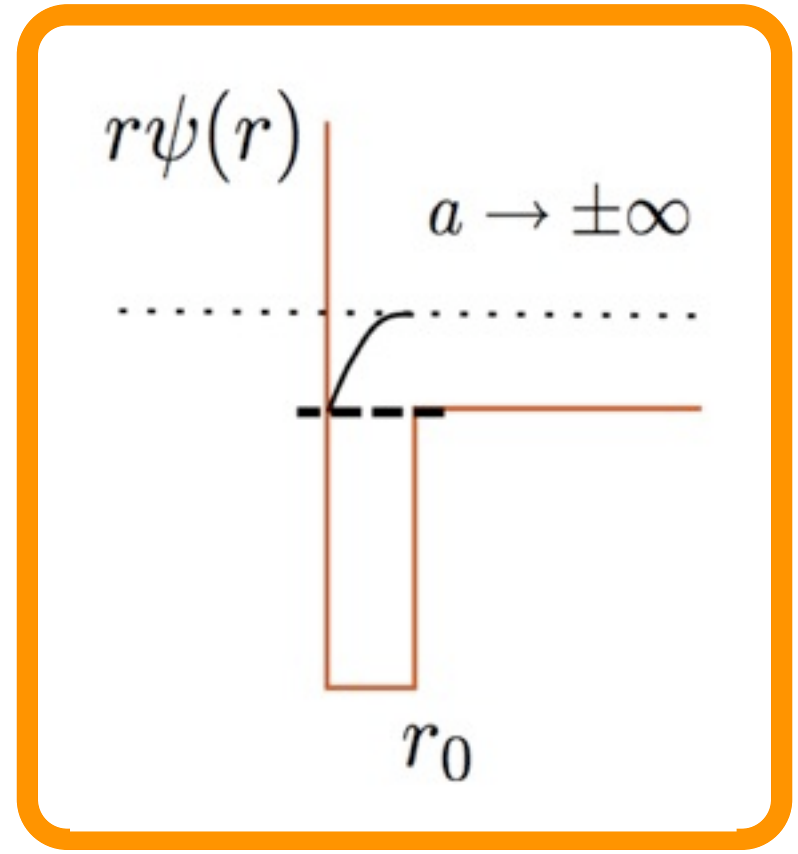
- Spin 1/2 fermions, at unitarity

$$r_0 \to 0 \ll n^{-1/3} \ll |a| \to \infty$$

Range of the interaction

Inter-particle distance

S-wave scattering length



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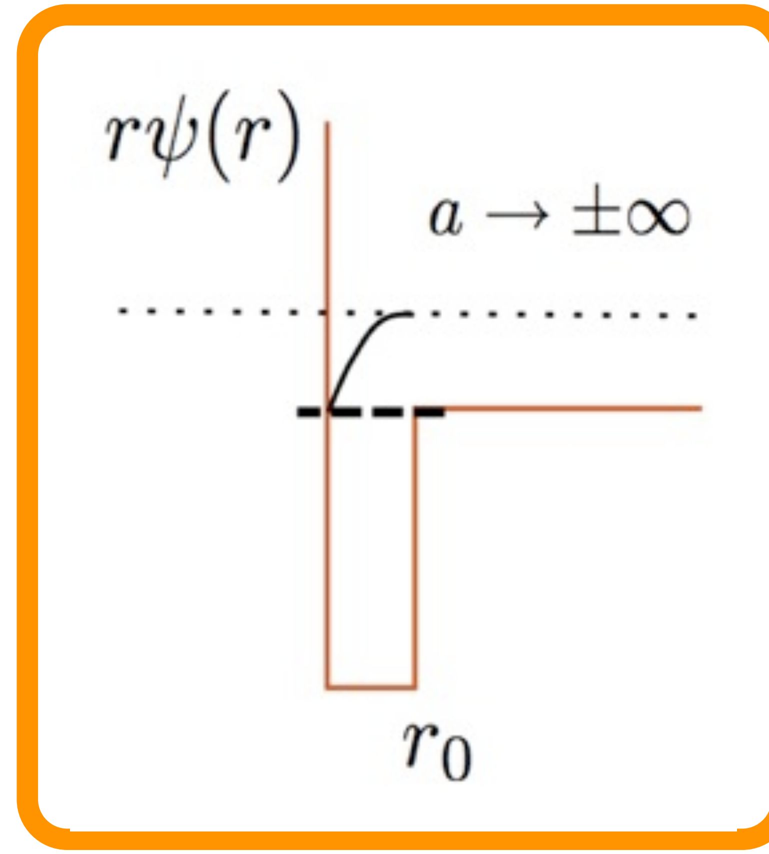

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- As many scales as a free gas!

$$k_F = \hbar(3\pi^2 n)^{1/3} \qquad \varepsilon_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{2/3}$$

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Every dimensionful quantity should come as a power of ε_F times a **universal** constant/function.

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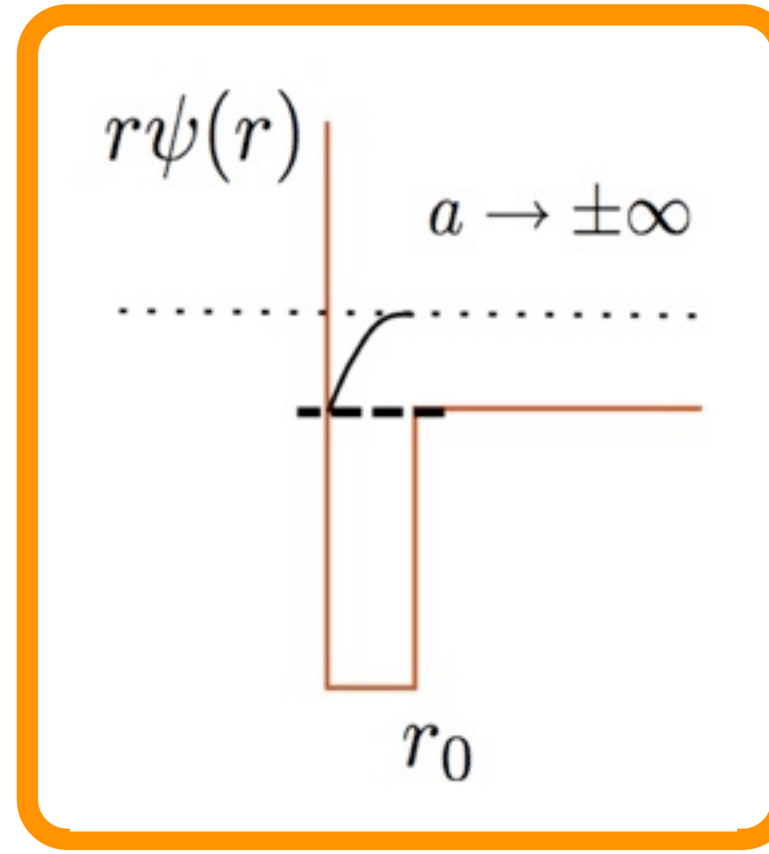

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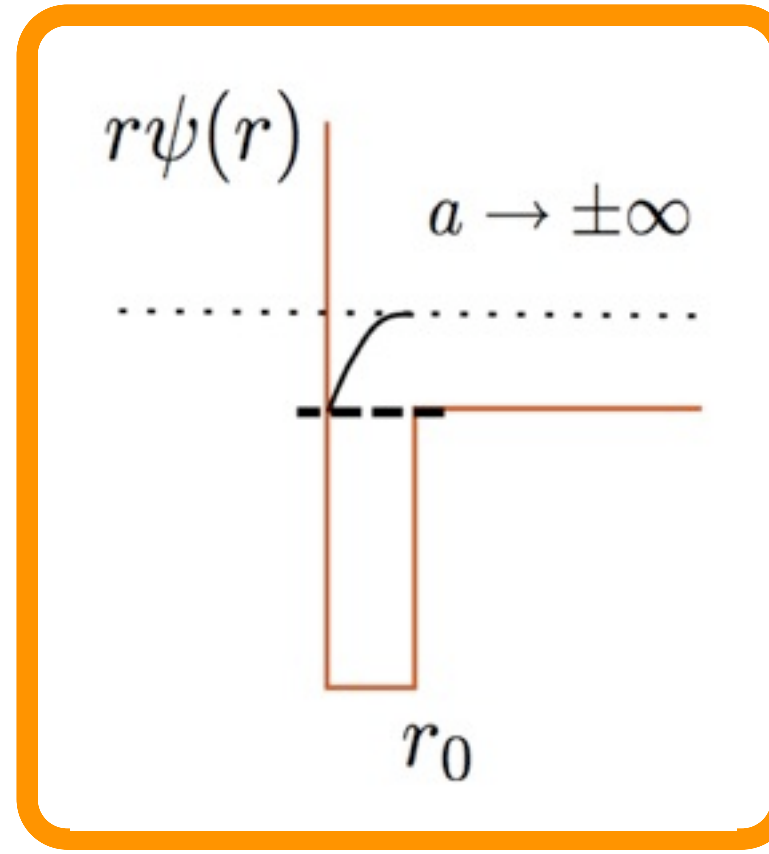

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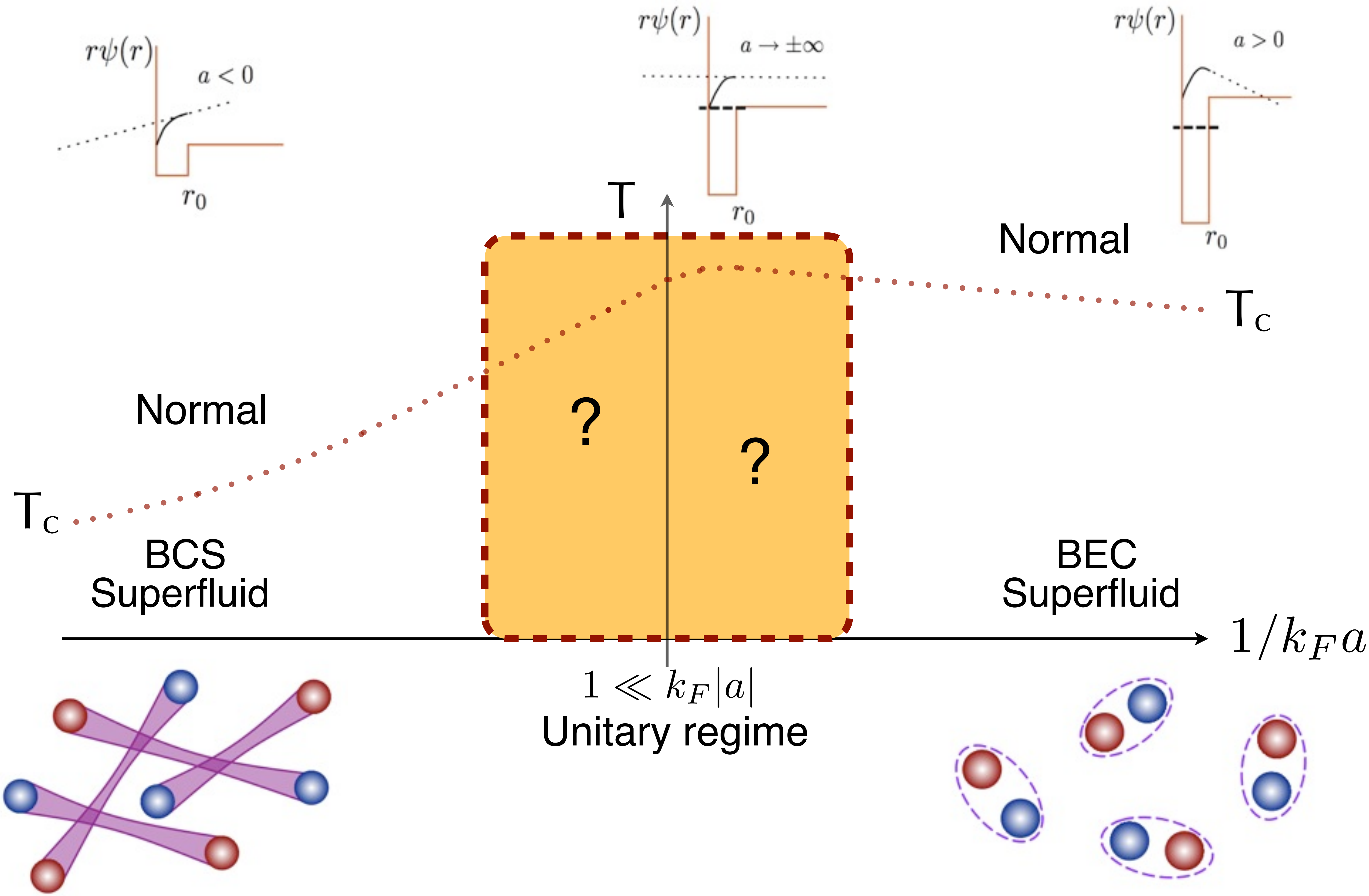
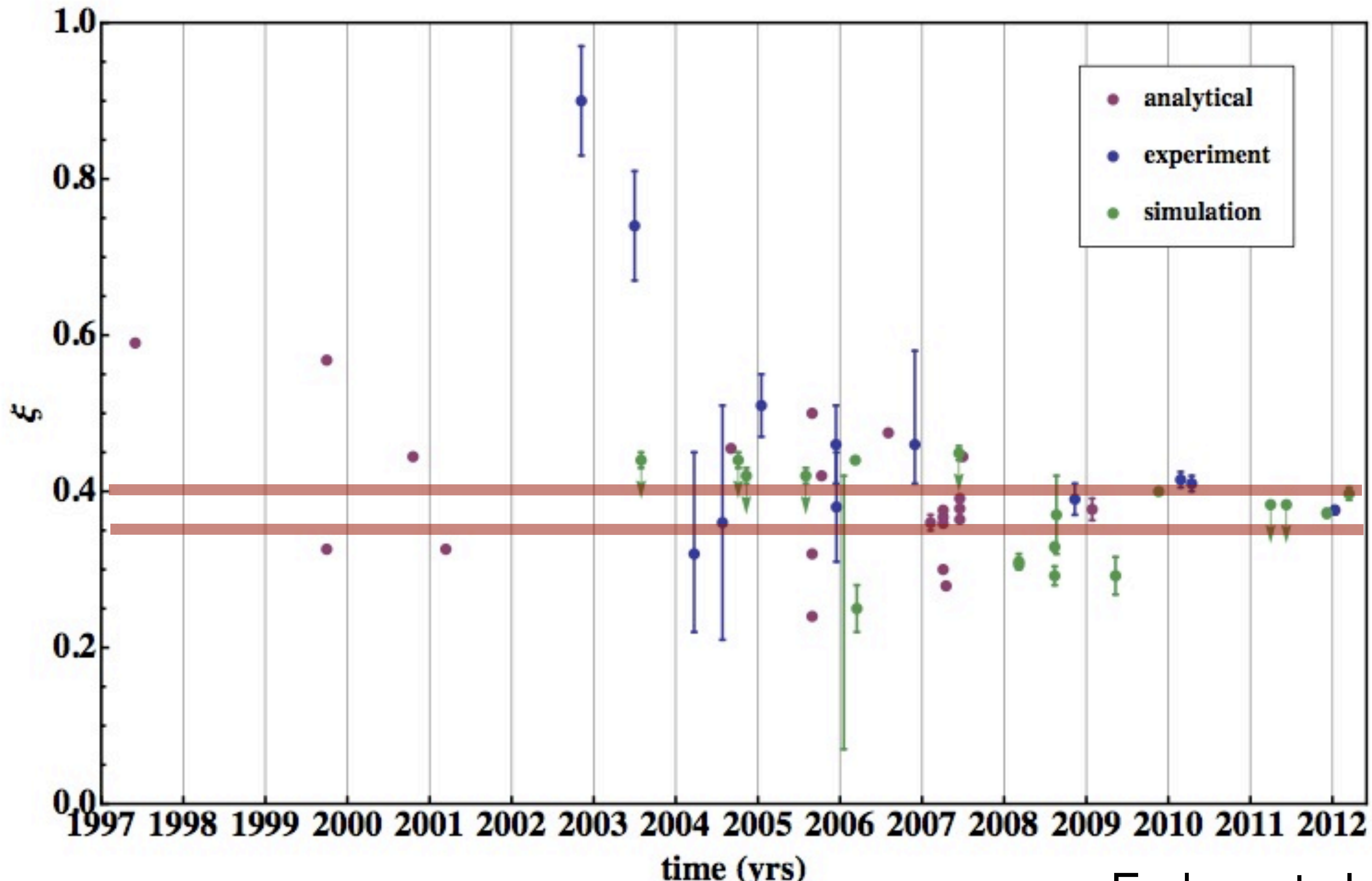
- Quantitatively **?**

The BCS-BEC Crossover



Energy update (ground state)

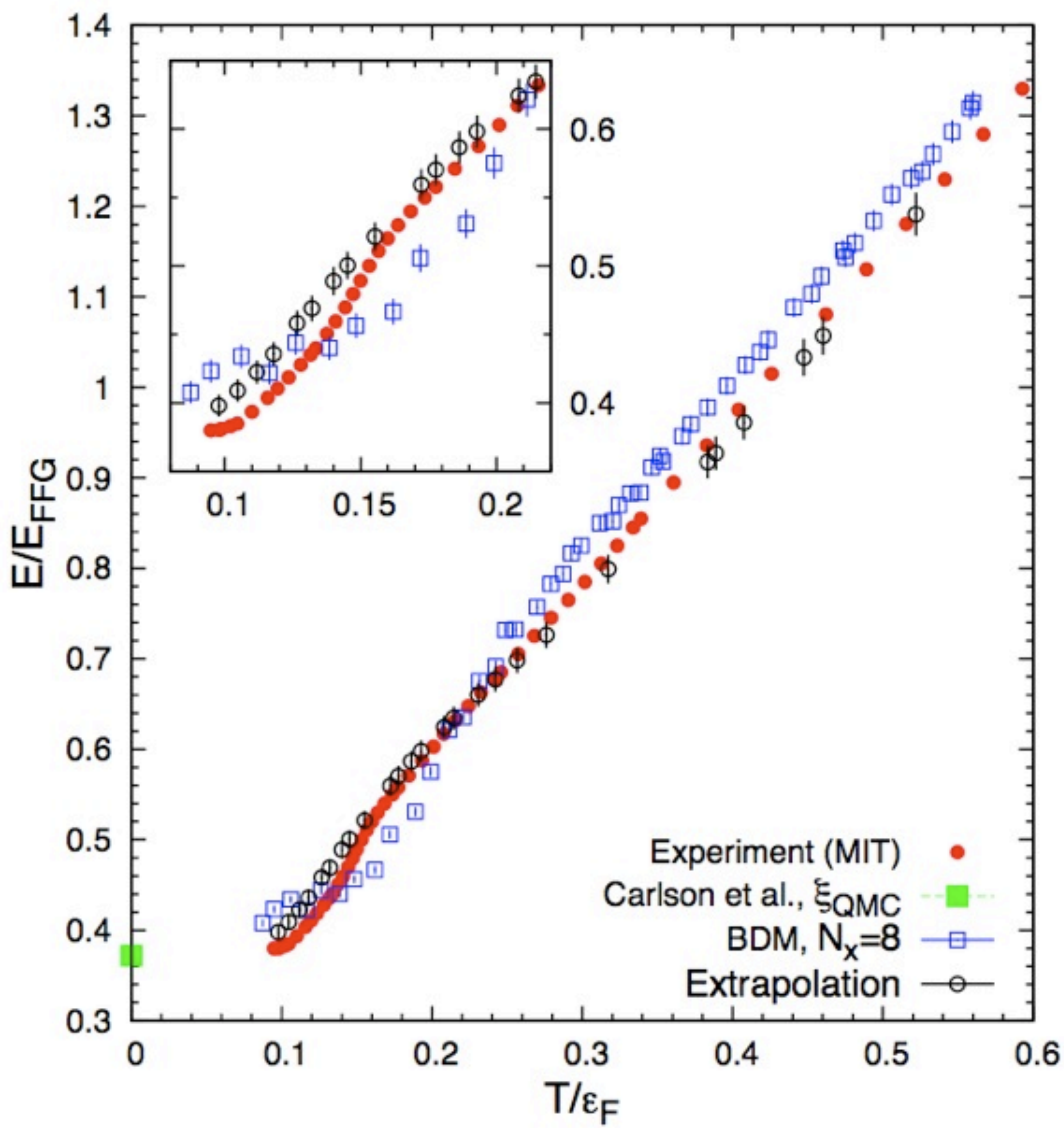
- Ground state energy per particle



Endres et al.

Energy update (finite temperature)

- Finite T equation of state (theory & experiment)



Experiment: Zwierlein et al. (MIT)

Drut, Lähde, Wlazlowski, Magierski, arXiv:1111.5079

Accepted PRA(R)

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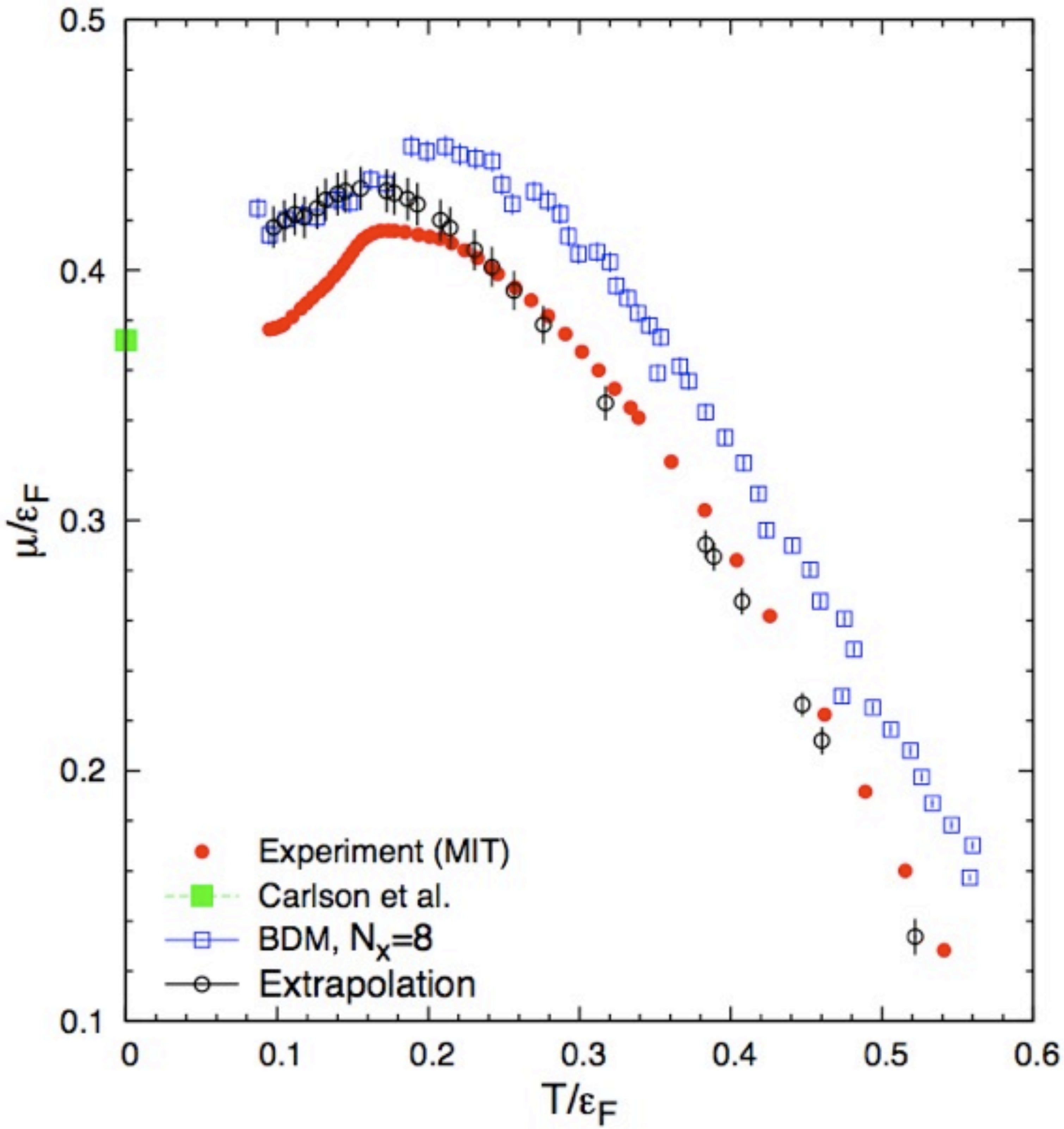

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The Tan relations and the "contact"

- Momentum distribution tail

$$n_k \underset{k \to \infty}{\longrightarrow} C/k^4$$

S. Tan, Annals of Physics **323**, 2952 (2008).

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- Energy relation

$$T + U = \sum_{\sigma} \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{\hbar^2 k^2}{2m} \left(n_\sigma(\boldsymbol{k}) - \frac{C}{k^4} \right) + \frac{\hbar^2}{4\pi m a} C$$

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- Short distance density-density correlator

$$\langle n_1(\boldsymbol{R} + \tfrac{1}{2}\boldsymbol{r})\, n_2(\boldsymbol{R} - \tfrac{1}{2}\boldsymbol{r}) \rangle \longrightarrow \frac{1}{16\pi^2} \left(\frac{1}{r^2} - \frac{2}{ar} \right) \mathcal{C}(\boldsymbol{R})$$

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- Adiabatic relation

$$\mathcal{C} = \frac{4\pi m a^2}{\hbar^2} \frac{\mathrm{d}\mathcal{E}}{\mathrm{d}a}$$

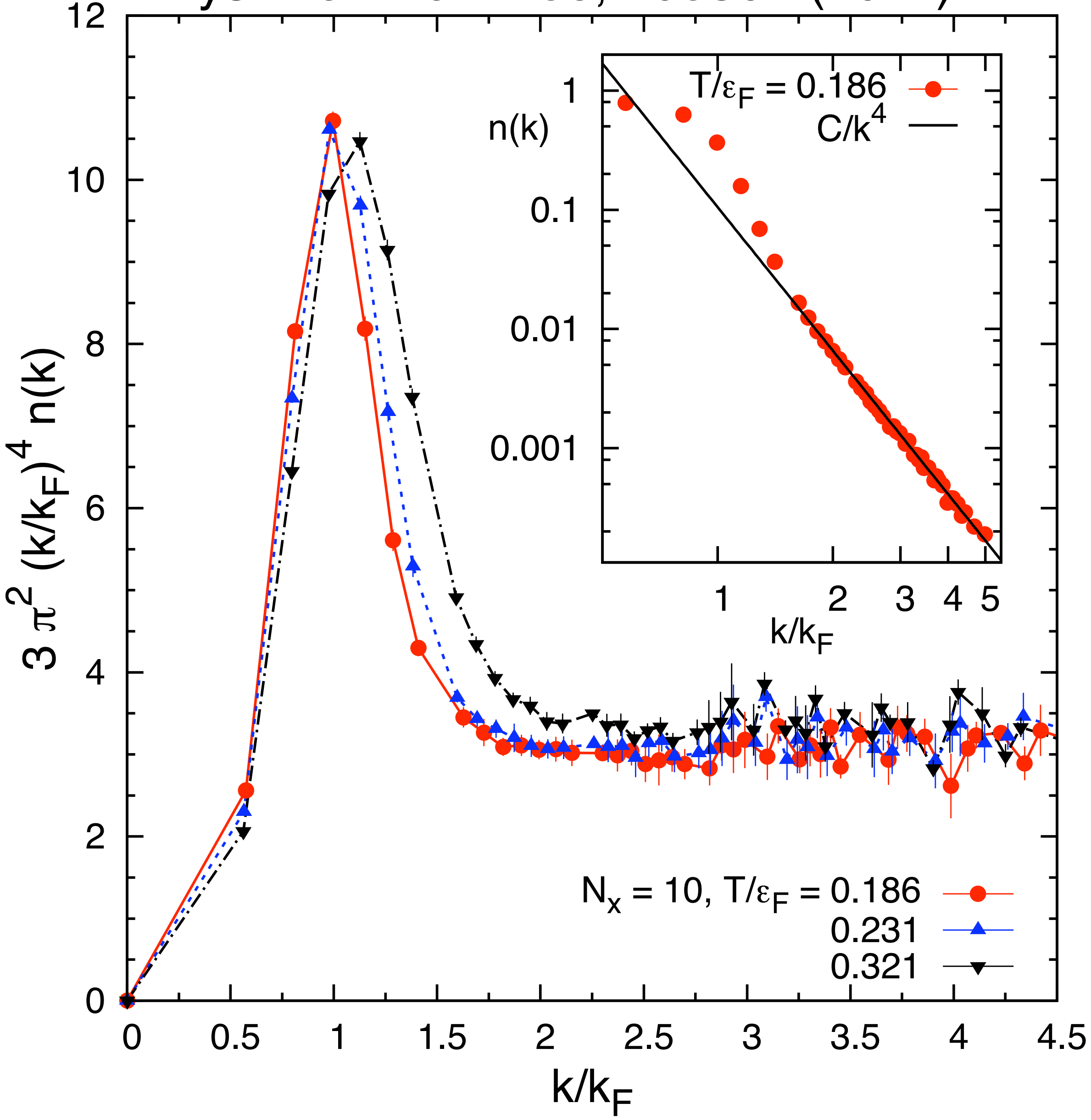
- Pressure relation

$$P = 2\varepsilon/3 + C/(12\pi m a)$$

Momentum distribution

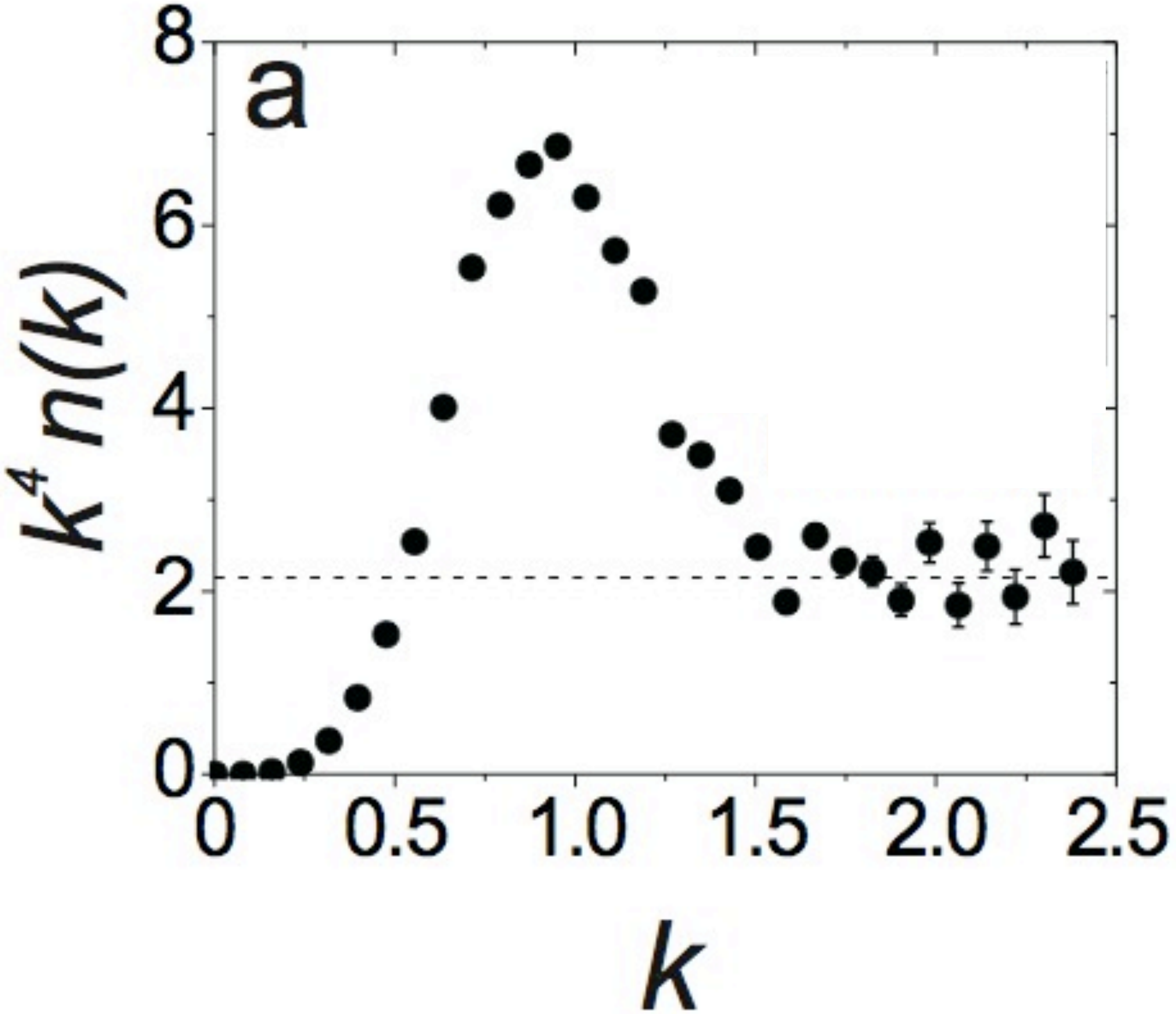
Theory (lattice)

J. E. Drut, T. A. Lähde, T. Ten
Phys. Rev. Lett. **106**, 205302 (2011)



Experiment

J. T. Stewart et al
PRL **104**, 235301 (2010)



- $T/T_F = 0 - 0.5$
- Plateau seen both in **theory** and **experiment**!

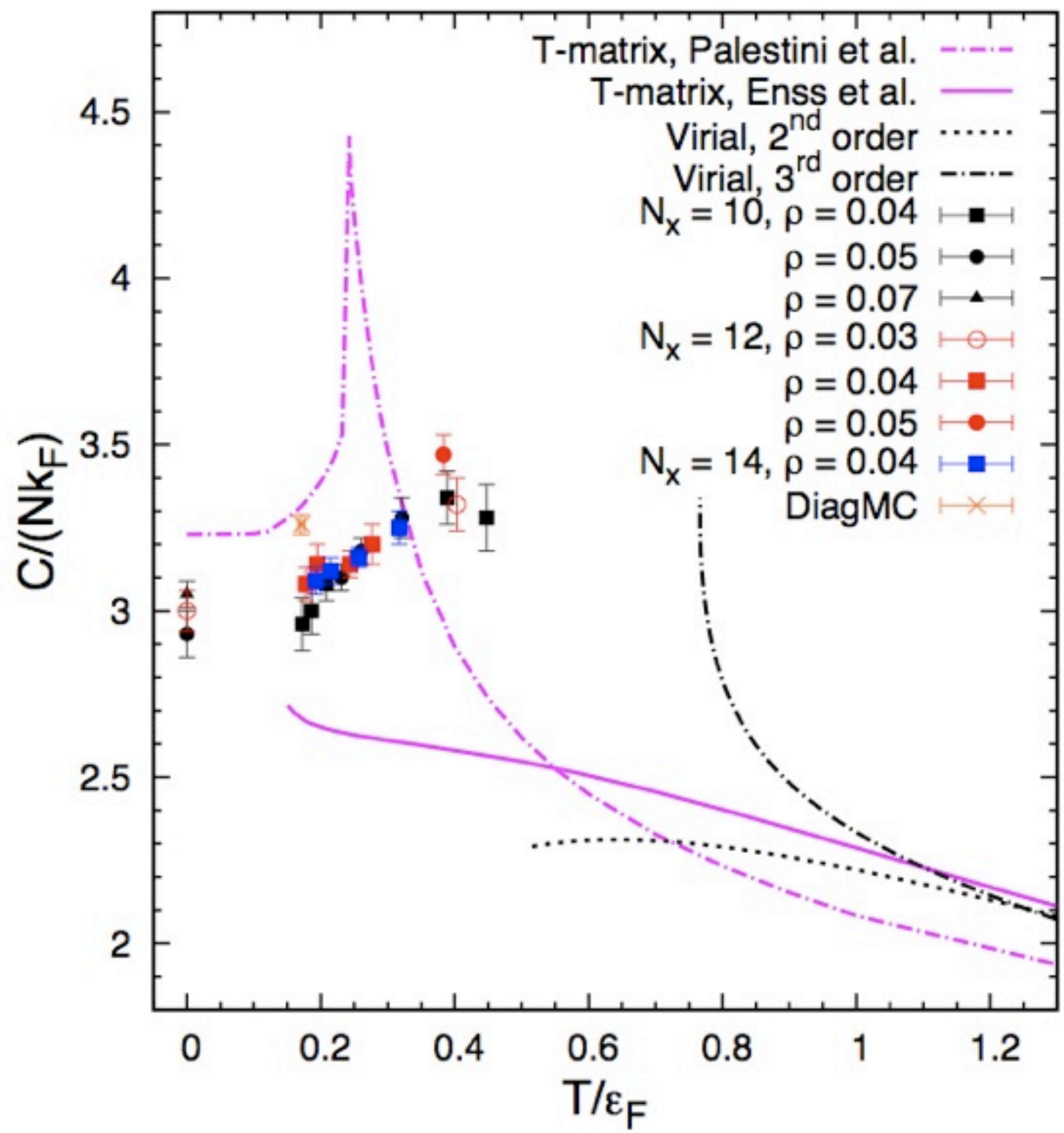
What do we know so far?

- Growth at low T
- Decrease at high T
- Maximum around T ≅ 0.4T_F
- Finite density effects?
- What happens in the crossover?

Virial expansion:
Yu, Bruun & Baym PRA **80**, 023615 (2009)
Hu, Liu, & Drummond, arXiv:1011.3845

T-matrix: Palestini et al.
PRA **82**, 021605 (2010)

Improved T-matrix: Enss et al.
`doi 10.1016/j.aop.2010.10.002`



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Recent technical developments

Dealing with systematic effects

- **Finite volume**
- **Finite lattice spacing**

→ **Related to each other**

Induce finite-range effects

In general we have... $$p\cot\delta(p) = -\frac{1}{a} + \frac{1}{2} r_{\mathrm{eff}} p^2 + O(p^4)$$

But we want... $p\cot\delta(p) \equiv 0$ **... at unitarity**

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→ **Can't do that with only one parameter!**

Effective range remains finite!

Point-like interaction

$$\hat{V} \equiv -g \sum_{i} \hat{n}_{\uparrow,i} \hat{n}_{\downarrow,i}$$

Transfer matrix

$$\mathcal{T} \equiv e^{-\tau \hat{H}} \simeq e^{-\frac{\tau \hat{T}}{2}} e^{-\tau \hat{V}} e^{-\frac{\tau \hat{T}}{2}} + O(\tau^2)$$

Dealing with systematic effects

We need a "richer" HS transformation

Endres et al. multiple papers.

Typically...

$$\mathcal{T} = \int \mathcal{D}\sigma \; \mathcal{T}_{\uparrow}[\sigma]\mathcal{T}_{\downarrow}[\sigma]$$

$$\mathcal{T}_s[\sigma] = e^{-\frac{\tau \hat{T}_s}{2}} \prod_{\boldsymbol{i}} \left(1 + \sqrt{A}\,\hat{n}_{s,\boldsymbol{i}} \sin\sigma_{\boldsymbol{i}}\right) e^{-\frac{\tau \hat{T}_s}{2}}$$

Now...

$$A(\mathbf{p}) = \sum_{n=0}^{N_{\mathcal{O}}-1} C_n \mathcal{O}_n(\mathbf{p})$$

$$\mathcal{O}_n(\mathbf{p}) = \left(1 - e^{-\mathbf{p}^2}\right)^n$$

$$\mathcal{O}_n(\mathbf{p}) = [2\sin(p/2)]^{2n}$$

Dealing with systematic effects

- **Highly improved actions**

  e.g. using Lüscher's formula

$$p\cot\delta = \frac{\mathcal{S}(E)}{\pi L}$$

s-wave phase shift

Energy eigenvalues in a box (no lattice)

$$\mathcal{S}(\eta) \equiv \lim_{\Lambda\to\infty} \sum_{\mathbf{n}} \frac{\Theta(\Lambda^2 - \mathbf{n}^2)}{\mathbf{n}^2 - \eta^2} - 4\pi\Lambda$$

$$\eta = \frac{pL}{2\pi}$$

$$E = p^2/m$$

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(scattering experiment information)

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→ Decide what scattering parameters you need

→ Tune your Hamiltonian accordingly

Dealing with systematic effects

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→ Decide what scattering parameters you need

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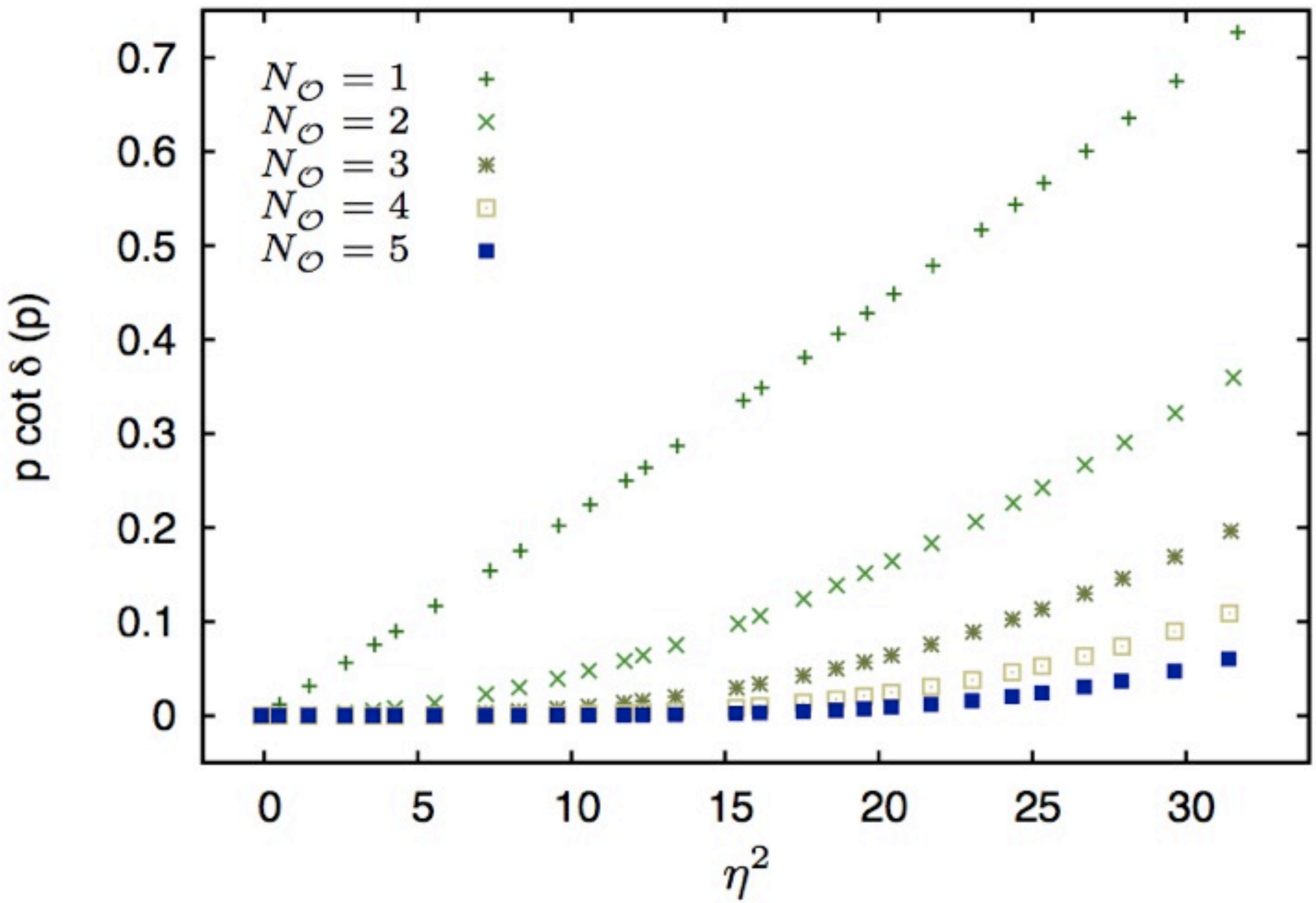
→ **Profit!**

Dealing with systematic effects

- **Highly improved actions**

  Adding more parameters to the transfer matrix and tuning via Lüscher's formula...



Improved transfer matrix

Endres et al. multiple papers.

JED arXiv:1203.2565

Dealing with systematic effects

- **Highly improved actions & operators**

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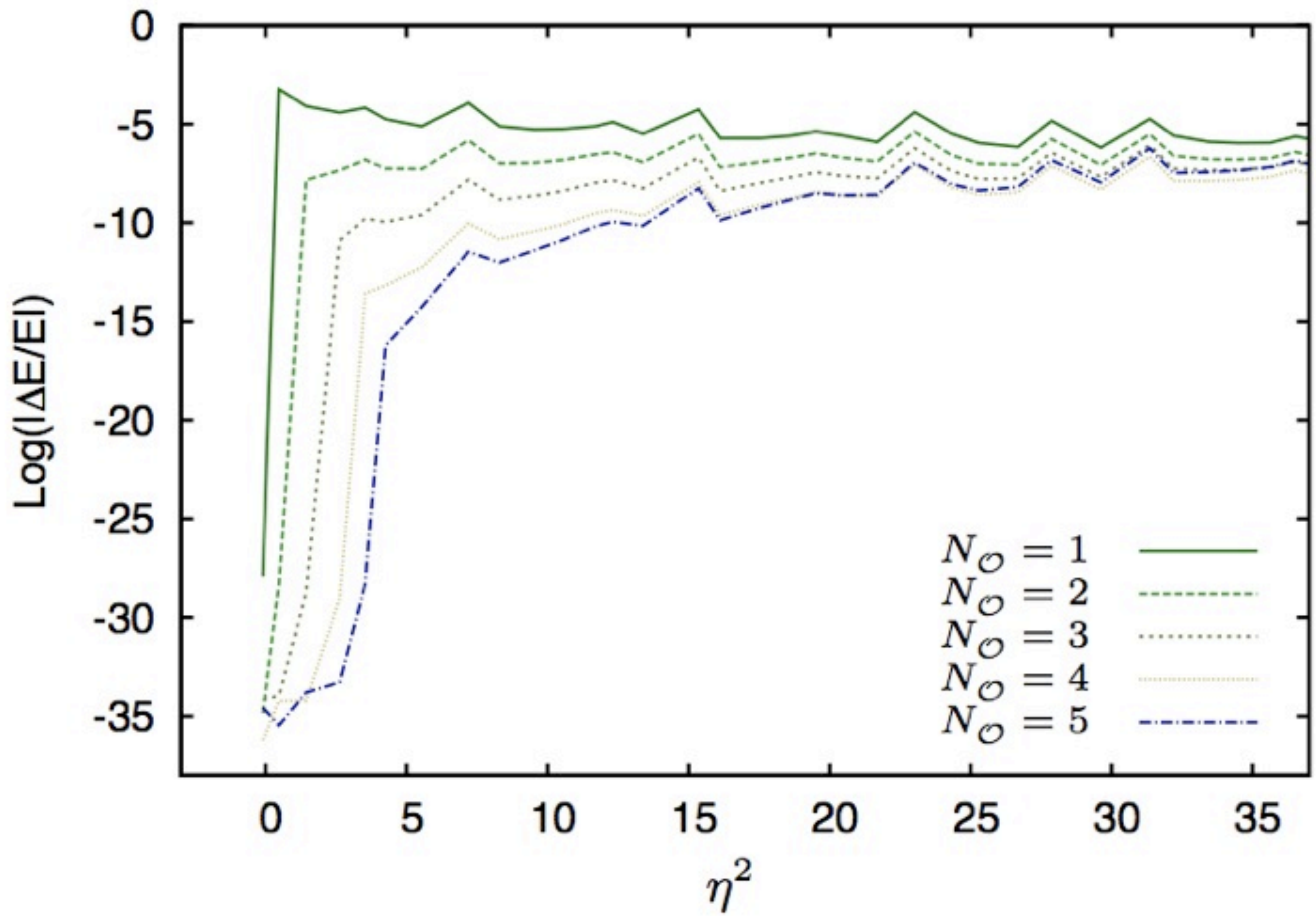

Energy

JED
arXiv:1203.2565

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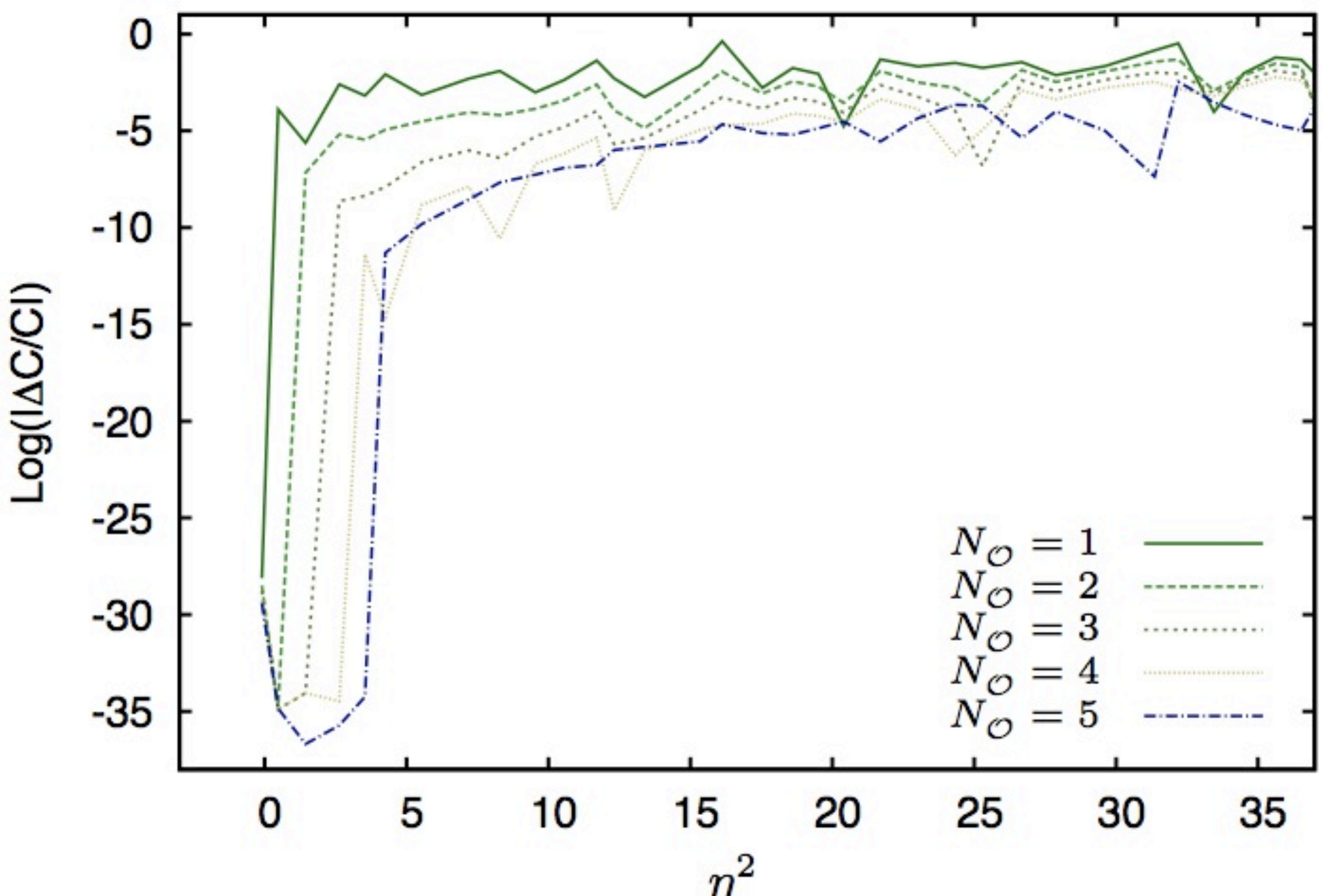


Contact

JED
arXiv:1203.2565

A more direct way to the contact...

At T=0...

$$\frac{\partial E}{\partial a^{-1}} = -\frac{\hbar^2}{4\pi m} C$$

At finite T...

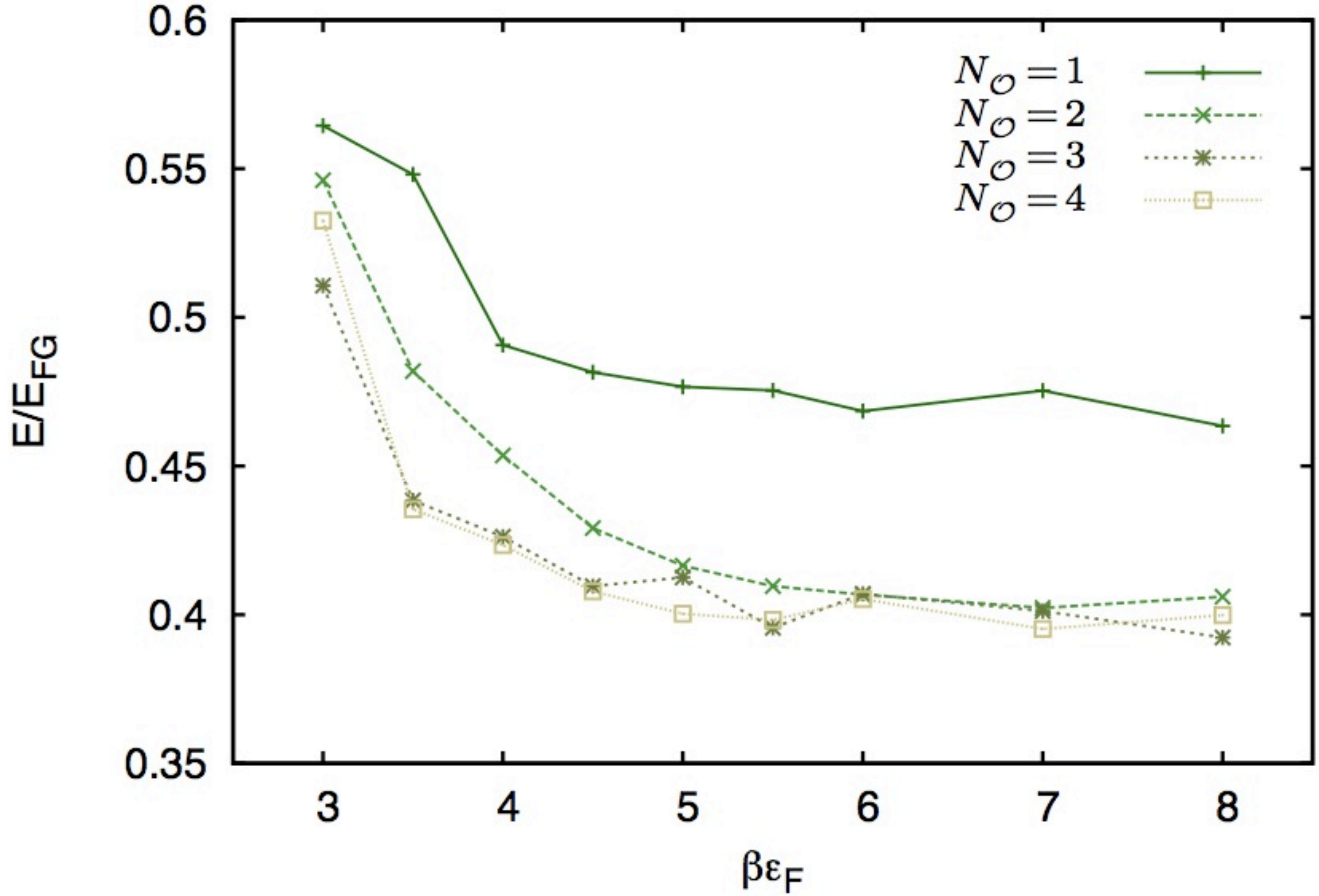
$$\left(\frac{\partial \Omega}{\partial a^{-1}}\right)_{T,\mu} = -\frac{1}{\beta}\left(\frac{\partial \log \mathcal{Z}}{\partial a^{-1}}\right)_{T,\mu} = -\frac{\hbar^2}{4\pi m} C$$

In both cases we need

$$\frac{\partial T_2^{\text{exact}}}{\partial a^{-1}} = -\tau \frac{\partial E_2}{\partial a^{-1}} \exp\left(-\tau E_2\right)$$

$$\frac{\partial E_2}{\partial a^{-1}} = -\frac{4\pi^3}{L}\left(\frac{d\mathcal{S}}{d\eta^2}\right)^{-1}$$

Results: GS Energy



JED
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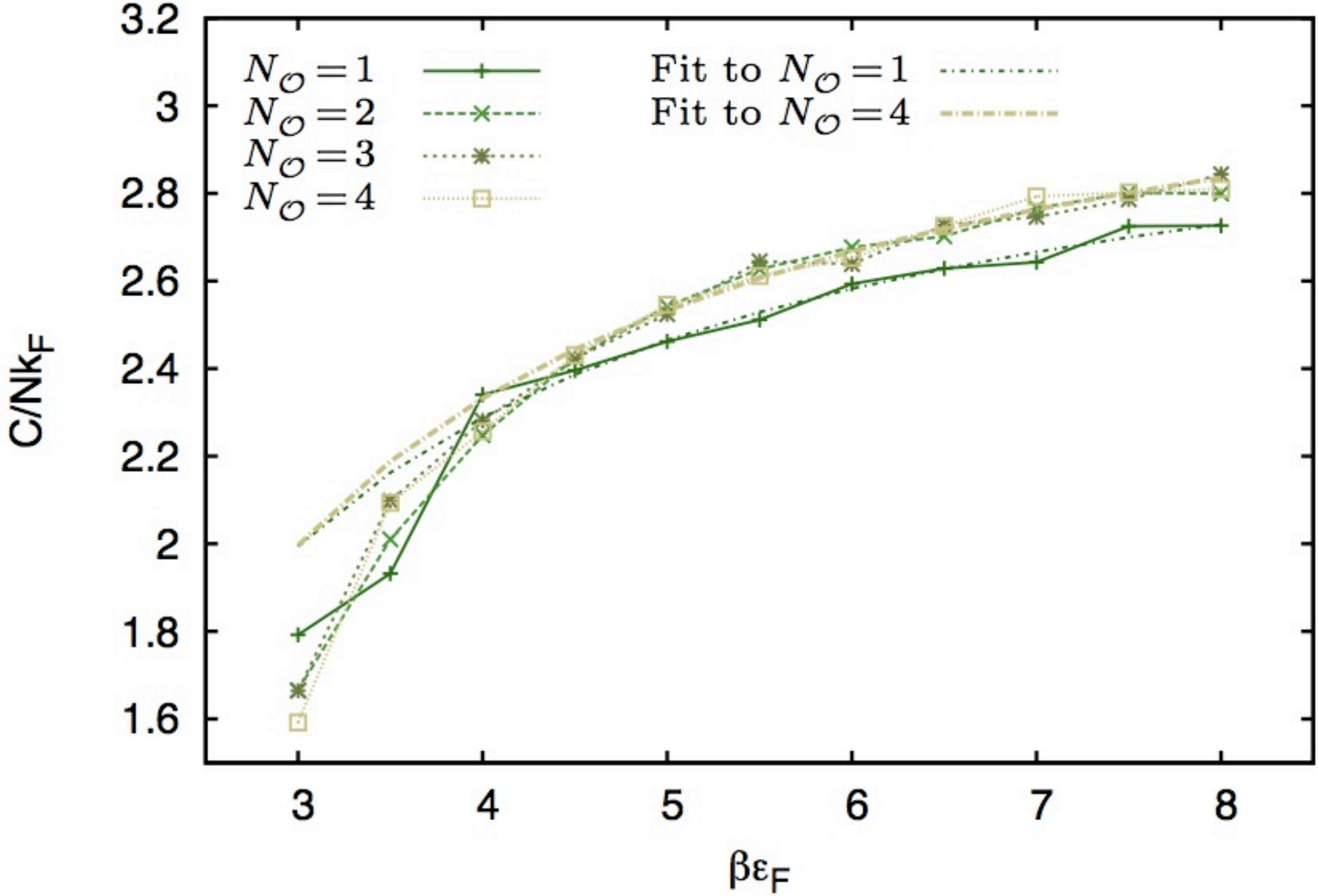
Results: GS Contact



JED
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Where do we go from here?

- We have implemented these improved actions and operators in our finite-temperature codes.
- We are reassessing our previous calculations in the light of new ones done with these new tools.
- We are simultaneously pursuing the calculation of response functions (specific heat, compressibility, susceptibility, viscosities).

Summary & conclusions

- Strongly interacting Fermi gases have **universal** properties
- Studying the universal regime **requires non-perturbative numerical approaches** such as Quantum Monte Carlo and Lattice QCD-type tools.
- Cond-mat, Nucl-th, Hep-th, Hep-lat are all interested in these problems! (again universality)

Summary & conclusions

- Strongly interacting Fermi gases have **universal** properties
- Studying the universal regime **requires non-perturbative numerical approaches** such as Quantum Monte Carlo and Lattice QCD-type tools.
- Cond-mat, Nucl-th, Hep-th, Hep-lat are all interested in these problems! (again universality)
- Much is known (much more than shown here) but much remains to be done! New tools are needed...
- Precise determination of equilibrium and linear-response quantities is largely in its infancy (just a couple of exceptions).
- Precision is required to understand the physics, in some cases even qualitatively!

We are entering a “precision” era!

Thank you!